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THEORY OF BIPOLARONIC BANDS

Vijay Kumar Pancholi

Department of physics , M.L.V Government college

Bhilwara, Rajasthan, India

ABSTRACT

For a two-orbital model with Jahn-Teller coupling to a two-fold degenerate phonon mode, we study the bipolaronic crossover as well as the pairing transition. The transition from weak to strong coupling is analogous to the behavior of the single-band Holstein model, which is as follows: When compared to the binding of bipolarons, which gives birth to a metal-to-insulator transition, the polaron crossover, in which electrons and phonons become tightly entangled, happens with a lower coupling. This results in the metal-to-insulator transition. It is interesting to note that a single bipolaronic transition takes place even though the two bands have dramatically different bandwidths. This is in contrast to the situation involving repulsive Hubbard-like interactions, for which it has been claimed that an orbital-selective Mott transition takes place. The inter-orbital character of the Jahn-Teller coupling is responsible for this phenomenon.

Keywords: *Bipolaronic, Bands, Interestingly*

INTRODUCTION

The explanation of the complex phase diagrams that are characteristic of highly correlated materials relies heavily on the interaction between spin, charge, and orbital degrees of freedom. This is because of the vital role that this interplay plays. The electron-phonon interactions, often known as e-ph interactions, are an essential mechanism that helps to describe the features of these systems. Most of the research that has been done on e-ph interactions has been confined to the Holstein model. This model proposes that the electronic state should form a band that is not degenerate, and that phonons should couple with the local electronic. On the other hand, many highly correlated materials feature d or f orbitals that are substantially identical to one another. By taking into account a degenerate electronic manifold and coupling it with the appropriate degenerate phononic models, we are able to go one step closer to providing a description of the e-ph interaction that occurs in these compounds that is more accurate. Because of the possible involvement of phonon dynamics in these narrow-band systems, the Born-Oppenheimer approximation is difficult to defend, and it is not possible to decouple the electronic orbital states from the vibrational modes.

The colossal magnetoresistance (CMR) compounds are a good example of a typical class of compounds that include such a spin-charge-orbital combination. In spite of the fact that the double-exchange mechanism is the foundation of the CMR phenomenon, which links the magnetic behavior to the conduction properties of a material, its interplay with the coupling between the degenerate eg electrons and the Jahn-Teller (JT) distortions of the MnO6 octahedra is crucial to describing the properties of these, which in turn lead to a variety of experimentally observed charge and/or orbital behaviors. The Jahn-Teller model is also applicable to the phenomenon of superconductivity in an alkali-doped AxC60 molecular solid. In this context, C60 refers to the fullerene molecule, while A denotes an alkali cation such as K, Rb, or Cs. The threefold degenerate

molecular level in the alkali-doped AxC60 is partially occupied, and it relates strongly to eight Hg intra-molecular levels. Jahn-Teller In these types of systems, the fact that crucial phonons have a JT nature has substantial repercussions when strong Coulomb forces are present.

When the charge excitations are locked by the Coulomb repulsion, the only degrees of freedom that are involved in the JT-driven interaction between the electrons are their spin and orbital degrees of freedom, and these degrees of freedom may still vary freely. Because of this, there is an increase in the phonon-induced superconductivity that is caused by correlation. In either scenario, it is the dynamic interplay between electron-electron and electron-phoenix interactions that has the potential to give rise to a wide range of physical events. In this study, we concentrate on the pure e-ph interaction term in order to emphasize the unique features given by orbital degeneracy before discussing the explicit involvement of electronic contacts. This is done in the same spirit as past examinations of the Holstein model, which focused on the same general question. For the same reason, which is that we want to capture the fundamental elements of the interaction between electrons and phonons, we do not permit superconductivity or chargedensity-wave ordering, which means that we are restricted to the normal state. It has been demonstrated that increasing the e-ph coupling in the half-filled Holstein model results in two processes that are coupled to one another yet take place in separate locations.

The first result is the well-known polaron creation, which may be defined as the gradual entanglement between the degrees of freedom of electronic motion and those of lattice motion. Polaron production does in fact occur as a continuous crossover, and one may locate it by evaluating the phonon displacement distribution function. This phenomenon can be traced back to its origin. An attraction is also induced between the fermions as a result of the attractive interactions. Even if superconductivity is purposefully suppressed, this will still result in the binding of fermionic carriers, which will ultimately cause a pairing transition, which, in the presence of polaronic carriers, will lead to a bipolaronic metal-insulator transition. In this study, we investigate the ways in which these physical principles are altered when applied to a Jahn-Teller model with two orbitals of e and E. For this scenario, we may additionally take into account various disturbances, such as the potential of differing bare widths for the two electronic bands. This idea is analogous to the much debated prospect of an orbital-selective Mott transition occurring in the context of repulsive Hubbard-like interactions. The document is structured as described below. In the next part, after briefly explaining the model and the technique of solution, we will begin to study the JT model at half-filling in and analyze how the e-ph coupling influences the electrical characteristics of the model. This will take place in the following section. After that, we investigate the topic of whether or not an orbital-selective bipolaron transition takes place in the system with varying band-widths. Following this, the final comments will be presented.

OBJEACTIVES

1. The study bipolaronic crossover and the pairing transition for a two-orbital model.
2. The study Interestingly, a single bipolaronic transition takes place also when the two bands.

RESEARCH METHODOLOGY

The $e \times E$. The Jahn-Teller model consists of two electron orbitals that are identical, as well as two phonon modes that are same,

$$
\begin{aligned}
H &= H_t + H_{ph} + H_{JT} \\
H_t &= -\sum_{\langle ij\rangle\gamma\sigma} t_\gamma (c^\dagger_{i\gamma\sigma} c_{j\gamma\sigma} + c^\dagger_{j\gamma\sigma} c_{i\gamma\sigma}) \\
H_{ph} &= \Omega_0 \sum_i (a_i^\dagger a_i + b_i^\dagger b_i) \\
H_{JT} &= g \sum_{i\sigma} [(n_{i1\sigma} - n_{i2\sigma})(a_i^\dagger + a_i) + \\
&+ (c^\dagger_{i1\sigma} c_{i2\sigma} + c^\dagger_{i2\sigma} c_{i1\sigma})(b_i^\dagger + b_i)],
\end{aligned}
$$

The model is solved via a technique known as dynamical mean field theory (DMFT). The method involves mapping the lattice model onto a quantum impurity model in which an interacting site is embedded into a non-interacting bath. The spectral function of the non-interacting bath needs to be determined self-consistently in such a way that the impurity Green's function of the quantum impurity model coincides with the local Green's function of the lattice model that is being considered in order to enforce a quantum dynamical mean-field theory. Because of this need, a self-consistency condition is reached, which stores information about the initial lattice in the form of the non-interacting density of states. The semi-circular density of states with a half-bandwidth D is a decision that is especially well-liked and helpful. $N(\omega) = \frac{2}{\pi D^2}\sqrt{D^2 - \omega^2}$. This corresponds to a Bethe lattice with an unlimited number of coordinations. The self-consistency equation for this system may be written in the following straightforward form:

$$
\frac{D^2}{4} G(i\omega_n) = \sum_k \frac{V_k^2}{i\omega_n - \epsilon_k},
$$

Already put to use in the investigation of highly correlated electron-phonon systems, the density functional theory (DMFT) has established itself as one of the most trustworthy techniques for the analysis of these systems. Research conducted on the normal phase of the Holstein model reveals that for e-ph couplings, the ground state is metallic with a Fermi liquid signature. However, when the coupling strength is increased, a first-order metal-insulator transition takes place. This phase exhibits a gap in the one-electron spectrum; however, in contrast to the metal-insulator Mott transition, neither hysteresis nor a preformed gap is observed for the transition from the metallic to the bipolaronic insulating phase, at least not for the relatively small values of phonon frequency that have been used. This is the case for the transition from the metallic to the bipolaronic insulating phase. The change from one kind of pairing to another is accompanied by the gradual entanglement of electronic and vibronic degrees of freedom, also known as the polaron crossover; however, this entanglement does not occur simultaneously with the pairing transition. Before the pairing transition can take place at relatively low phonon frequencies, polarons will have already been produced. Because the subsequent take transition binds two polarons, it is possible to refer to this transition as a bipolaronic transition. An important objective of this study is to determine whether or whether the symmetry of the e-ph coupling may have an effect on the electrical properties and the dynamic characteristics of a particular system and, if so, to what degree this can occur.

DATA ANALYSIS

First, we will concentrate on the isotropic systems that have bands that are all the same, written as D1 = D2 = D. In addition, we restrict ourselves to the adiabatic regime with a small ratio of the phonon frequency to the

semi-bandwidth (0 = 0.2D1), which is a domain in which the dynamics of phonons are sluggish in comparison to the usual kinetic energy of electrons. In this regime, we have a small ratio of the phonon frequency to the semi-bandwidth. We present the quasi-particle weight zi z as a function of the electron-phonon coupling constant. These findings were achieved for this particular example when the electron-phonon coupling constant was at half-filling. When the coupling constant is increased in a system that has e-ph interaction, that system will enter a strong-coupling polaronic regime. This is the kind of regime in which the presence of an electron is linked with a finite lattice distortion.

When the system is operating in the polaronic domain, it is characterized by low-energy excitations that, although being severely renormalized, nonetheless maintain their coherence. Additionally, the same e-ph coupling may be responsible for a pair of polarons with opposing spins being attracted to one another and producing a bound state in real space that is referred to as a bipolaron. In DMFT, those pairs are unable to move, and the production of bipolarons leads to a transition from a metal to an insulator. This transition is related with the divergence of the effective mass as well as the disappearance of a coherent peak at the Fermi level at a critical coupling gc. This process is evident in our DMFT results from the enhancement of the electron effective masses, and the corresponding reduction of the quasi-particle weights as the e-ph coupling constant g increases. This process eventually reaches the bipolaronic metal-insulator transition (MIT), which is shown in panel (a) of Figure (1). Figure 1 presents the double occupancies (d1 = d2) as a function of the value of g in its panel (b). Around the critical coupling, gc, there is a significant rise in the number of double occupancies, which demonstrates a first order transition into the bipolaronic phase.

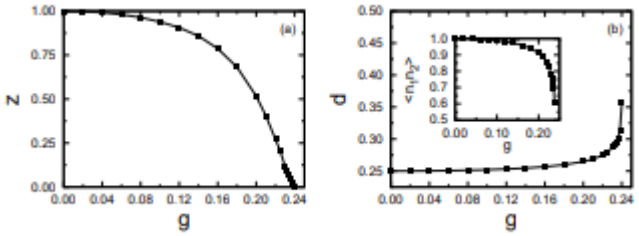

FIG. 1: Panel (a): The quasi-particle weights, z1 = z2, at half-filling as a function of electron-phonon interaction, g. Panel (b): double occupancy, d1 = d2, as a function of g. The inset of the panel (b) shows the orbital correlation, hn1n2i, between the two orbitals.

The polaron crossover is not evident in the evolution of the quasi-particle weights or the double occupancies. As a result, we have estimated the phonon displacement probability distribution function in order to shed light on this particular issue. demonstrate how the phonon displacement probability distribution function, P(x), changes as a function of the gravitational constant g. In the case of isotropic systems, the point spread functions (PDFs) for the a-mode and the b-mode are identical. When the e-ph coupling is increased, there is a smooth transition that takes place between a unimodal distribution and a bimodal distribution. This behavior is a full analogue to the single-band Holstein model.

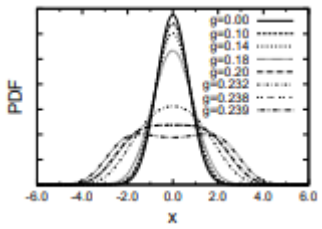

FIG. 2: Phonon displacement distribution function P(x). The various lines correspond to different values of g.

Before entering the bipolaronic phase, which is defined by z = 0, there is a very limited area in which polarons are generated; nonetheless, the value of the quasi-particle weights, although being extremely tiny, are different from zero (see two dot-dashed curves). This occurs before the bipolaronic phase enters. The presence of this zone demonstrates that, in the process of the metal-insulator bipolaronic transition, bipolarons are created for those values of g that are considerably bigger than the polaron crossover. This is shown by the fact that the existence of this region is seen. In the Jahn-Teller model, the qualitative conclusion is comparable to what was discovered for the Holstein model; however, the area in which polarons may exist without giving rise to bipolarons is shown to be far more constrained. Up to this point, we have spoken about the bipolaronic transition for the electrical system with two orbitss that has the same bandwidth.

The degeneracy of the valence bands, on the other hand, is commonly lifted as a consequence of the geometric complexity of many transition metal oxides, which gives birth to coexisting partly filled narrow- and wide-bands. This is because of the fact that many transition metal oxides have a common structure. It has been shown that in a certain range of repulsive Coulomb interactions and Hund's coupling the so-called orbital-selective phase occurs, in which the narrow-band is insulating while the wide-band is still metallic. In actuality, the two-band Hubbard model with orbitals of different widths has recently received a considerable amount of attention. In this model, there are two sets of orbitals, each with a different width. In the scenario of a phonon interaction including the complete charge on the two orbitals, as in a generalized Holstein model, the situation would most likely be comparable to the scenario of the repulsive Hubbard model. This is because both scenarios include the whole charge on the two orbitals. In point of fact, a Holstein coupling causes a charge-charge attraction, which, in the antiadiabatic limit 0, reduces to an attractive Hubbard model. This model, in turn, is identical to the repulsive one when the system is half-filled. Instead, the answer to this issue is not readily apparent for the JT interaction. This is due to the fact that the phonon modes are not connected to the overall charge; rather, they are associated with the orbital degrees of freedom. In particular, the b-mode is inextricably linked to a hybridization between the two orbitals, an effect that works in direct opposition to the behavior of an orbital selector. We get a slowed attraction as a result of integrating out the phonons in our effective action, in which the interaction element of is present exclusively on the impurity.

On the other hand, the increase in the number of sites that are occupied by two people at the same time is contingent not only on the band but also on the value of the bandwidth ratio. The tight band quickly creates a higher number of spots that are held by two different people, and the impact becomes more dramatic as the band becomes even smaller. When the ratio D2/D1 is decreased, the crucial value of g for the transition from metal to insulator also drops. This behavior is pretty predictable given that we are maintaining D1 at its previous level while decreasing D2. Because of this, the overall kinetic energy of the system is decreased, which makes the formation of polarons and bipolarons simpler (both the polaron crossover and the bipolaron

transition are expected to occur because the e-ph interaction overcomes the kinetic energy and its delocalizing effect, at least in the adiabatic regime, in which the energetic convenience also implies a sizeable entanglement) (both the polaron crossover and the bipolaron transition are expected to occur because the The phonon displacement distribution functions may be seen at the following location: The various behaviors of the two phonon modes are determined by the breaking of the symmetry that exists between the two orbitals.

The probability density function of the a mode becomes bimodal prior to the bipolaronic transition as the e-ph coupling strength grows, but for the same values of the coupling, the PDF remains unimodal. Until the bipolaron transition, the PDF of the b-mode maintains its unimodal form, with a single feature that broadens without displaying any signs of bimodality. This is true all the way up to the point when the bipolaron transition occurs. It was discovered that the two peaks of the bimodal distribution for the a mode had somewhat varying heights from one another. When compared to the scenario in which bandwidths are same, the breadth of the area of couplings between the polaron crossover for the a mode and the metal insulator transition is much bigger.

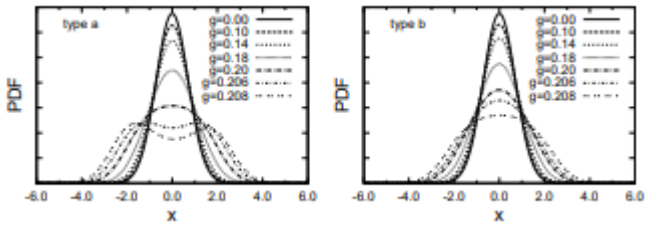

FIG. 3: Phonon displacement distribution function P(x). The left panel is for a phonon mode which shows bimodality. The right panel is for b phonon mode which does not show bimodality.

CONCLUSION

When the charge excitations are frozen by the Coulomb repulsion, the only degrees of freedom that are still free to vary are the spin and orbital degrees of freedom. In fact, the JT-driven interaction between the electrons only involves these two degrees of freedom. Because of this, there is an increase in the superconductivity that is driven by correlations rather than phonons.In either scenario, it is the dynamic interplay between electron-electron and electron-phoenix interactions that has the potential to give rise to a wide range of physical events. In this study, we concentrate on the pure e-ph interaction term in order to emphasize the unique features brought about by orbital degeneracy before discussing the explicit involvement of electronic contacts. This is done in the same vein as prior explorations of the Holstein model, which was developed by Holstein. For the same reason, which is that we want to capture the fundamental elements of the interaction between electrons and phonons, we do not permit superconductivity or chargedensity-wave ordering, which means that we are restricted to the normal state. It has been demonstrated that increasing the e-ph coupling in the half-filled Holstein model results in two processes that are coupled to one another yet take place in separate locations.

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